Single Crystal Si Nanowires Can Not Conduct the Heat

Investigator: P. Yang, UC-Berkeley

The observed thermal conductivity of single-crystalline silicon nanowires (sub 10 W/m.K for 20 nm wire) is more than *two orders of magnitude* smaller than the bulk value. This strong size-dependent thermal conductivity in these wires can be ascribed to the increased role of boundary phonon [lattice vibration] scattering. This thermoconductivity study in nanostructures is not only of fundamental theoretical interest since they will demonstrate the unusual phonon transport phenomena caused by the size confinement effects, but also of application significance since today's microelectronic devices are quickly moving into the sub-100 nm regimes and the corresponding thermal design urgently needs experimental data for sub-100 nm structures. The reduced thermal conductivity in semiconductor nanowires is greatly desired in applications such as thermoelectric cooling and power generation, but is not preferable for other applications such as electronics and photonics.

Reference: D. Y. Li, Y. Wu, R. Fan, P. D. Yang, A. Majumdar *Appl. Phys. Lett. 83*, 3186 – 3188 (2003).

Single Crystal Si Nanowires Can Not Conduct the Heat

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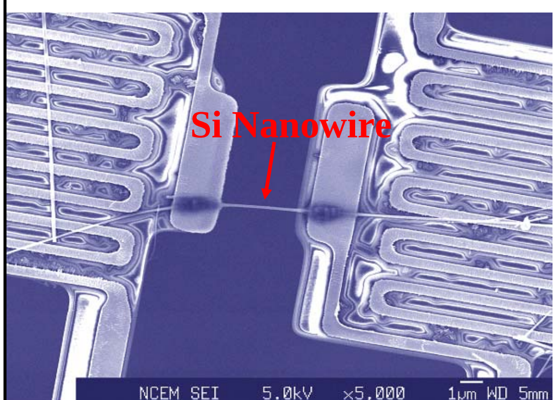
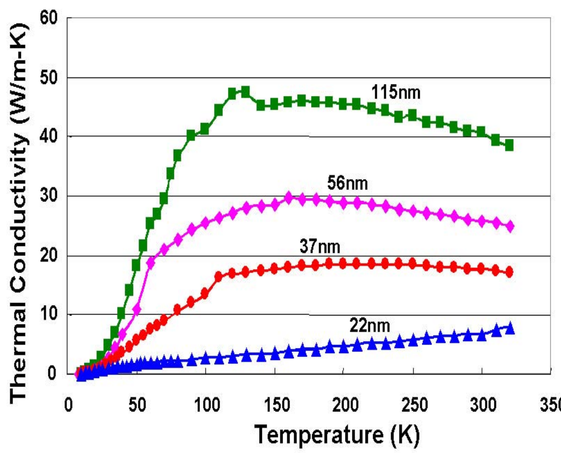


Suspended Nanowire device for Thermoconductivity measurement

Size-dependent thermoconductivity



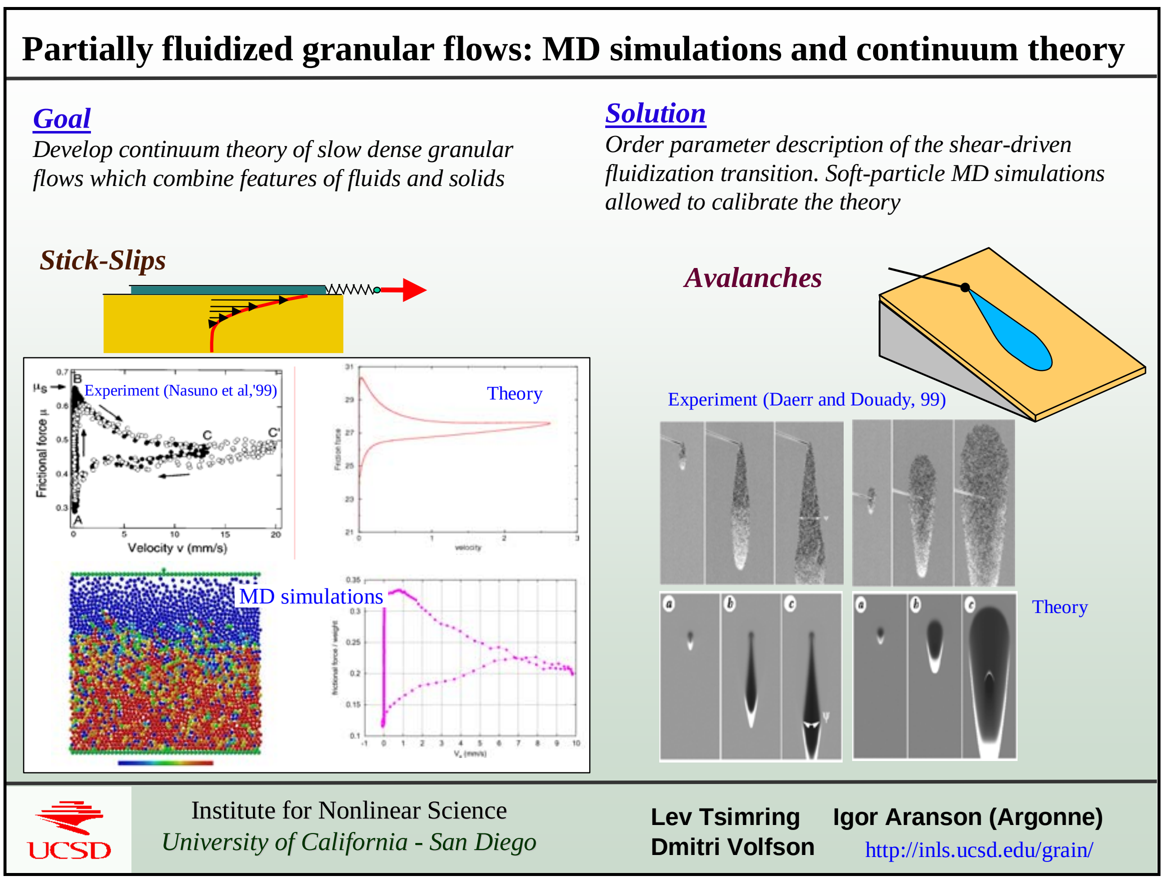
Majumdar & Yang, *Appl. Phys. Lett. 83*, 3186 (2003).

Granular Flows: Are They Solids, Liquids or Both?

Investigator: L. Tsimring, UCSD and I. Aranson, ANL

A continuum theory of partially fluidized granular flows has been developed. It successfully explains several important problems with industrial significance including: avalanches, granular friction, stick-slip dynamics, and near-surface shear flow. Unlike dilute granular flows which can be well described by the kinetic theory of granular gases, dense slow granular flows exhibit properties of solids and fluids simultaneously. The new theory directly deals with this major problem by explicitly incorporating both solid and fluid phases in the constitutive relation. The key ingredient of the theory is the separation of the shear stress into a “fluid part” proportional to the strain rate, and a remaining “solid part” supported by force chains. Continuum description of granular flows is of paramount importance for reliable and efficient engineering design of equipment for handling granular solid materials. Industrial applications may include pharmaceuticals, food, coal, agriculture, and construction.

Reference: I.S.Aranson and L.S.Tsimring, *Phys.Rev. E*, 64, 020301 (2001); I.S.Aranson and L.S.Tsimring, *Phys. Rev. E*, 65, 061303 (2002); D.Volfson, L.S.Tsimring and I.S.Aranson, *Phys. Rev. Letters*, 90, 254301(2003); and, D.Volfson, L.S.Tsimring and I.S.Aranson, *Phys. Rev. E,* 68, 021301 (2003).



Do Nanofluids Conduct as Much Heat as They Should?

Investigators: D. Cahill and P. Braun, U. Illinois

Nanoscale composites or nanofluids are under intense investigation for applications as novel thermal management fluids and materials. Certain suspensions of nanoscale colloidal metal particles as well as of carbon nanotubes in fluids exhibit anomalous enhancements in the thermal conductivity. Picosecond time-scale measurements of time-resolved transient absorption have been used to make the first quantitative measurements of heat transfer at the solid/fluid interface using laser techniques. These experiments directly investigate the thermal coupling between particles and the surrounding fluid and rule-out explanations based on enhanced heat transport in the fluids near the particle surface. But even larger improvements would be expected based on simple theory and the high thermal conductivity and high aspect-ratio of carbon-nanotubes. These results explain why the predicted improvements in thermal conductivity are not observed: the thermal coupling between the nanotube and the surrounding matrix is weak, greatly impeding heat transfer in the carbon-nanotube composite. The results also indicate that the interface thermal conductance is highly sensitive to the structure and chemistry of the particle/fluid interfaces.

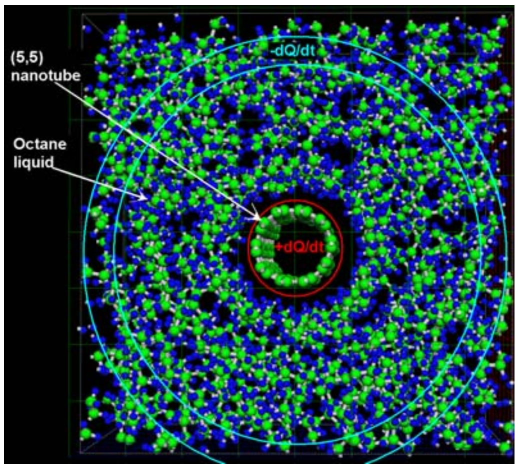
Reference: S. T. Huxtable, *et al.*, *Nature Materials* (in press).

Do nanofluids conduct as much heat as they should?

D. Cahill, M. Strano, P. Braun
Frederick Seitz Materials Research Laboratory

P. Keblinski,
Rensselaer Polytechnic Institute

Adding small quantities of carbon nanotubes to a fluid produces a dramatic increase in its ability to carry heat. However, theory predicts a much larger enhancement than is observed. Reasons for this discrepancy, revealed by direct comparisons of optical measurements and computer simulations carried out on picosecond time scales, are that the thermal coupling between nanotubes and the surrounding fluid is poor. This work advances the design of new thermal management technologies—ones fully exploiting the properties of advanced nanomaterials.



Computer model of a carbon nanotube surrounded by a hydrocarbon liquid. The thermal coupling predicted by the simulation is in good agreement with experiments.

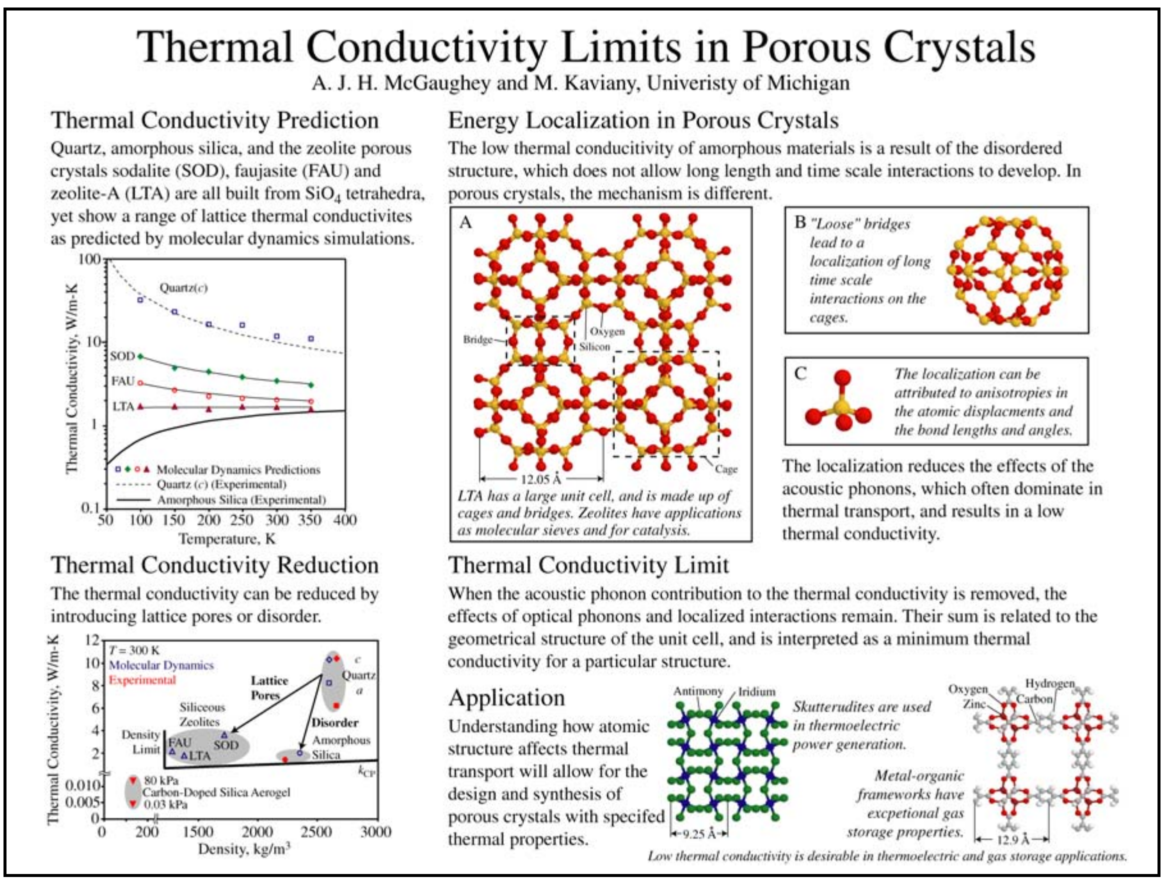
ILLINOIS

Thermal Conductivity Limits in Porous Crystals

Investigators: M. Kaviany & A. McGaughey, U. Michigan

The thermal transport behavior of porous crystals has importance to variable temperature application ranging from thermoelectric power generation to hydrogen storage in automobiles. By using molecular dynamics simulations to identify atomic level heat transfer mechanisms, the very low room temperature lattice (phonon) thermal conductivity (~ 1 W/m-K) of the zeolite porous crystals has been explained. It was found that the cage-bridge structure of these materials results in local distortion and anisotropy of atomic bond lengths and angles effectively eliminating the potentially large contribution of the acoustic phonons [lattice vibrations] to the thermal conductivity. Heat transfer in these cases is only realized through short range optical phonons and localized interactions. This later situation is interpreted as a lower limit to crystalline thermal conductivity and it indicates that the arrangement of the atoms in a given structure is critical to its thermal transport behavior. This understanding of how atomic structure affects thermal transport will allow for new porous crystals (such as the metal-organic frameworks and the skutterudites) to be designed and synthesized with exceptionally low thermal conductivities.

Reference: A. J. H. McGaughey and M. Kaviany, *International Journal of Heat and Mass Transfer* (2 articles in press).



Can Superconducting Magnets Take the Stress?

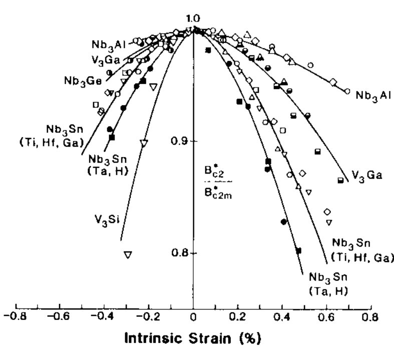
Investigators: J. Ekin, National Institute for Standards and Technology and D. Welch, Brookhaven National Laboratory

A large, reversible stress induced degradation of the critical parameters of practical superconductors strongly affects the design of superconducting magnets for high-energy physics particle accelerators, industrial magnets and magnetic resonance imaging systems used in medical applications. Until know, the origin of this degrading effect has not been understood, and methods for predicting its magnitude have been elusive. Recently, however, a strong correlation was discovered between the magnitude of the stress effect and the degree of phonon anharmonicity, or softness, of the crystal lattice of the superconductor. A model was developed which explains this correlation and several phenomena, including the stress insensitivity of entire classes of superconductor materials and the effects of alloying additions on the stress effect. This discovery also led to several predictions, including new methods to change the stress sensitivity and parameters (internal friction, phonon softening, and third-order elastic constants) for predicting the effect in previously untested systems. The overall effect is a fundamental breakthrough in understanding the origin of one of the dominant factors limiting the performance and utilization of commercial superconducting magnets and cables, which may also impact new designs for transformers and power conditioning equipment in the electric power-utility industry.

Can Superconducting Magnets Take the Stress?

A large, reversible strain degradation of the critical properties of practical superconductors strongly affects the design of superconducting magnets for high-energy physics accelerators, industrial magnets, and MRIs in health diagnostics. Until now, the origin of this effect has not been understood. A strong correlation has been found between the magnitude of the strain effect and the degree of phonon anharmonicity, or softness, of the superconductor's crystal lattice. This has resulted in a fundamental breakthrough in understanding the origin and predicting mechanical limits for the performance of practical superconducting machinery.

Superconducting generator, subjecting superconductors to 0.25% axial strain, 10^4 g transverse loads, and fatigue.



Significantly reduced axial-strain effect in Nb_3Al compared with Nb_3Sn superconductors.

J. Elkin (NIST) and D. Welch (BNL)